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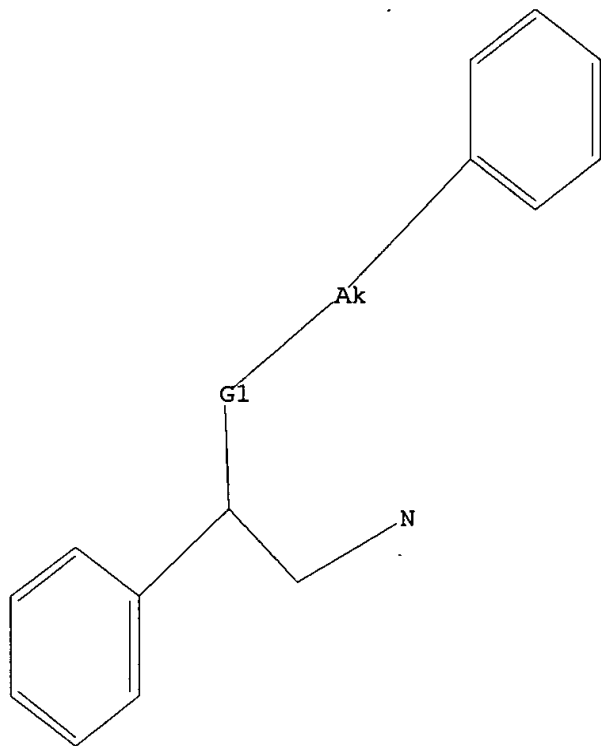
Uploading 09912163 (patel).str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 O,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam

SAMPLE SEARCH INITIATED 08:04:35 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 16607 TO ITERATE

6.0% PROCESSED 1000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

20 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 324434 TO 339846  
PROJECTED ANSWERS: 5549 TO 7735

L2 20 SEA SSS SAM L1

=>

Uploading 09912163 (patel).str

L3        STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3        STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s 13 sss sam

SAMPLE SEARCH INITIATED 08:05:56 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 14120 TO ITERATE

7.1% PROCESSED        1000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    \*\*COMPLETE\*\*

BATCH    \*\*COMPLETE\*\*

PROJECTED ITERATIONS:        275291 TO    289509

PROJECTED ANSWERS:                0 TO        0

L4        0 SEA SSS SAM L3

=> s 13 sss ful

FULL SEARCH INITIATED 08:06:09 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 281248 TO ITERATE

100.0% PROCESSED    281248 ITERATIONS

81 ANSWERS

SEARCH TIME: 00.00.15

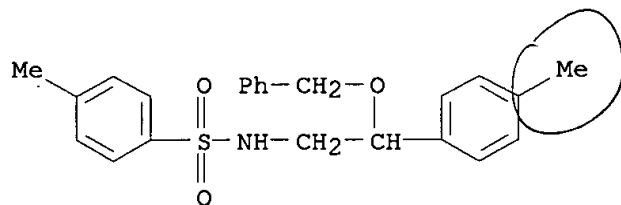
L5        81 SEA SSS FUL L3

=> s 15

L6        13 L5

=> d 16 1-13 bib,ab,hitstr

L6 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2003 ACS  
 AN 2002:483428 CAPLUS  
 DN 137:384426  
 TI Montmorillonite clay catalyzed cleavage of aziridines with alcohols  
 AU Yadav, J. S.; Reddy, B. V. S.; Balanarsaiah, E.; Raghavendra, S.  
 CS Division of Organic Chemistry, Indian Institute of Chemical Technology,  
 Hyderabad, 500007, India  
 SO Tetrahedron Letters (2002), 43(29), 5105-5107  
 CODEN: TELEAY; ISSN: 0040-4039  
 PB Elsevier Science Ltd.  
 DT Journal  
 LA English  
 OS CASREACT 137:384426  
 AB A variety of N-tosyl aziridines react smoothly with alcs. in the presence  
 of montmorillonite KSF or Amberlyst-15 at ambient temp. to afford the  
 corresponding .beta.-amino ethers in excellent yields with high  
 selectivity.  
 IT **476171-15-0P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of .beta.-amino ethers by montmorillonite catalyzed cleavage of  
 aziridines with alcs.)  
 RN 476171-15-0 CAPLUS  
 CN Benzenesulfonamide, 4-methyl-N-[2-(4-methylphenyl)-2-(phenylmethoxy)ethyl]-  
 (9CI) (CA INDEX NAME)

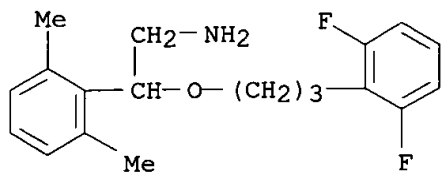


RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2003 ACS  
 AN 2002:157723 CAPLUS  
 DN 136:216523  
 TI Preparation of phenylethanol(mono/di)amines and  
 phenylalkylethanol(mono/di)amines as sodium channel blockers  
 IN Fuchs, Klaus; Stransky, Werner; Grauert, Matthias; Carter, Adrian; Gaida,  
 Wolfram; Weiser, Thomas; Ensinger, Helmut  
 PA Boehringer Ingelheim Pharma K.-G., Germany  
 SO PCT Int. Appl., 73 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA German  
 FAN.CNT 1

*Appl. Pat*

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002016308	A1	20020228	WO 2001-EP9036	20010804
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	DE 10040901	A1	20020314	DE 2000-10040901	20000818
	US 2002042410	A1	20020411	US 2001-912163	20010724 ←
	AU 2001091737	A5	20020304	AU 2001-91737	20010804
	EP 1311471	A1	20030521	EP 2001-971870	20010804
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
PRAI	DE 2000-10040901	A	20000818		
	US 2000-228675P	P	20000829		
	WO 2001-EP9036	W	20010804		
OS	MARPAT 136:216523				
AB	Title compds. [I; R1 = OH, CF3, NO2, CN, halo, C1-8 alkyl, halo, C1-8 alkoxy; R2, R3, R4 independently = halo, C1-8 alkyl, OH, NO2, CN, C1-8 alkoxy, CF3; R5, R6 independently = C1-8 alkyl, C2-8 alkenyl, C3-8 alkynyl, C3-8 cycloalkyl, NH2, OH, O, COOH, CONH2; A = C1-5 alkylene, C2-4 alkenylene, C3-4 alkylene; X = NH, N(CHO), halo, O, etc.] are prepd. The invention further relates to a method for producing said compds. and to their compn. in use as medicaments. Title compds. I are used as blockers of the voltage-dependent sodium channel and can be used for diseases that are assocd. with a functional disorder caused by hyperexcitability. Thus, the title compd. II was prep. from trifluoroacetic anhydride, 2,6-dimethylbenzaldehyde, which was prepd. from 2-bromo-3-dimethylbenzene, and 2-(3-bromopropyl)-1,3-difluorobenzene, which was prepd. from di-Et malonate and 2,6-difluorobenzyl bromide.				
IT	<b>401938-15-6P</b> RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of phenylethanolamines and phenylalkylethanolamines as sodium channel blockers)				
RN	401938-15-6 CAPLUS				
CN	Benzeneethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl-(9CI) (CA INDEX NAME)				



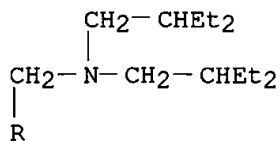
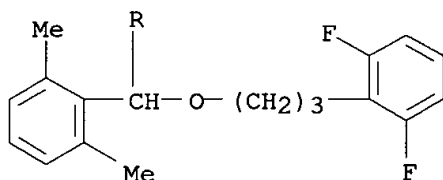
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 401938-23-6P 401938-29-2P 401938-31-6P  
 401938-33-8P 401938-35-0P 401938-36-1P  
 401938-38-3P 401938-42-9P 401938-45-2P  
 401938-49-6P 401938-51-0P 401938-53-2P  
 401938-55-4P 401938-57-6P 401938-59-8P  
 401938-61-2P 401938-63-4P 401938-67-8P  
 401938-69-0P 401938-71-4P 401938-73-6P  
 401938-75-8P 401938-77-0P 401938-79-2P  
 401939-43-3P 401939-45-5P 401939-49-9P  
 401939-51-3P 401939-53-5P 401939-54-6P  
 401939-55-7P 401939-56-8P 401939-58-0P  
 401939-60-4P 401939-62-6P 401939-64-8P  
 401939-66-0P 401939-68-2P 401939-70-6P  
 401939-72-8P 401939-74-0P 401939-76-2P  
 401939-78-4P 401939-80-8P 401939-82-0P  
 401939-84-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of phenylethanamines and phenylalkylethanamines as sodium channel blockers)

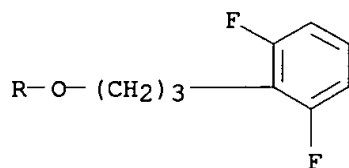
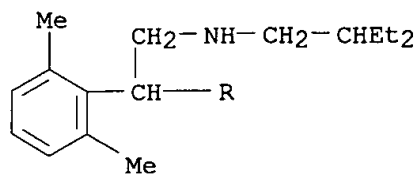
RN 401938-17-8 CAPLUS

CN Benzenethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-N,N-bis(2-ethylbutyl)-2,6-dimethyl- (9CI) (CA INDEX NAME)



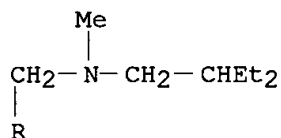
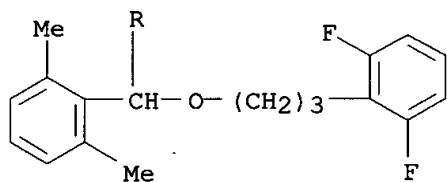
RN 401938-19-0 CAPLUS

CN Benzenethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-N-(2-ethylbutyl)-2,6-dimethyl- (9CI) (CA INDEX NAME)



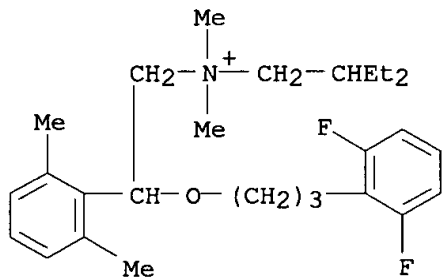
RN 401938-21-4 CAPLUS

CN Benzeneethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-N-(2-ethylbutyl)-N,2,6-trimethyl- (9CI) (CA INDEX NAME)



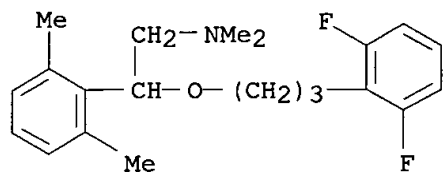
RN 401938-23-6 CAPLUS

CN Benzeneethaninium, .beta.-[3-(2,6-difluorophenyl)propoxy]-N-(2-ethylbutyl)-N,N,2,6-tetramethyl-, iodide (9CI) (CA INDEX NAME)

I<sup>-</sup>

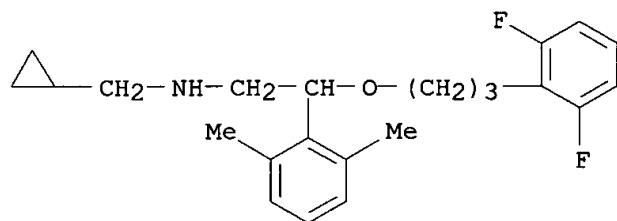
RN 401938-29-2 CAPLUS

CN Benzeneethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-N,N,2,6-tetramethyl- (9CI) (CA INDEX NAME)



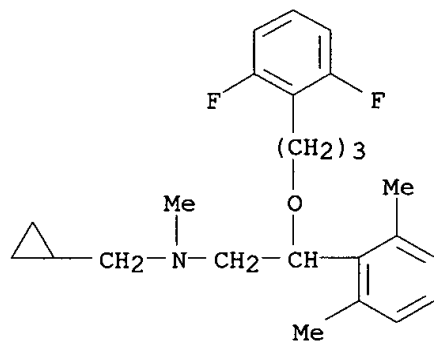
RN 401938-31-6 CAPLUS

CN Benzeneethanamine, N-(cyclopropylmethyl)-.beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl- (9CI) (CA INDEX NAME)



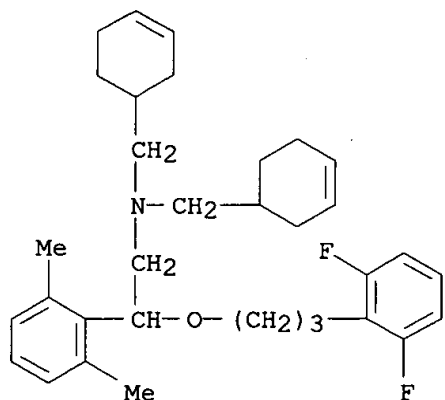
RN 401938-33-8 CAPLUS

CN Benzeneethanamine, N-(cyclopropylmethyl)-.beta.-[3-(2,6-difluorophenyl)propoxy]-N,2,6-trimethyl- (9CI) (CA INDEX NAME)



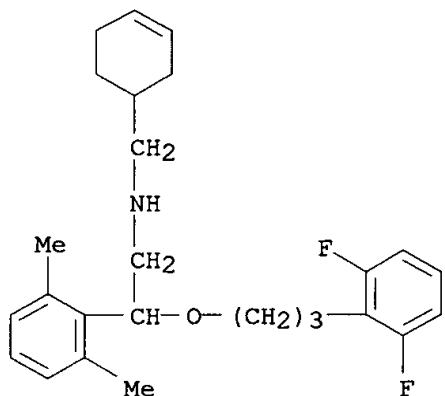
RN 401938-35-0 CAPLUS

CN Benzeneethanamine, N,N-bis(3-cyclohexen-1-ylmethyl)-.beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl- (9CI) (CA INDEX NAME)



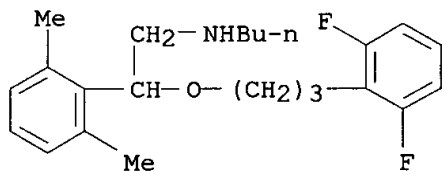
RN 401938-36-1 CAPLUS

CN Benzeneethanamine, N-(3-cyclohexen-1-ylmethyl)-.beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl- (9CI) (CA INDEX NAME)



RN 401938-38-3 CAPLUS

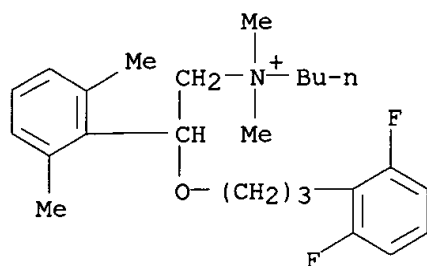
CN Benzeneethanamine, N-butyl-.beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl- (9CI) (CA INDEX NAME)



RN 401938-42-9 CAPLUS

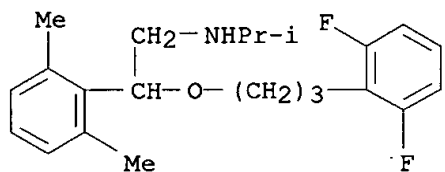
CN Benzeneethanaminium, N-butyl-.beta.-[3-(2,6-difluorophenyl)propoxy]-N,N,2,6-tetramethyl-, iodide (9CI) (CA INDEX NAME)





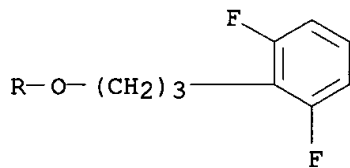
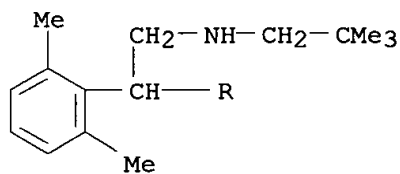
RN 401938-45-2 CAPLUS

CN Benzeneethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl-N-(1-methylethyl)- (9CI) (CA INDEX NAME)



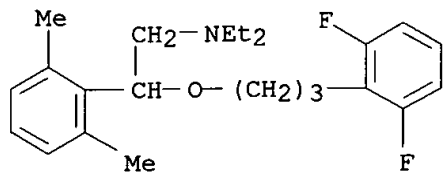
RN 401938-49-6 CAPLUS

CN Benzeneethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-N-(2,2-dimethylpropyl)-2,6-dimethyl- (9CI) (CA INDEX NAME)



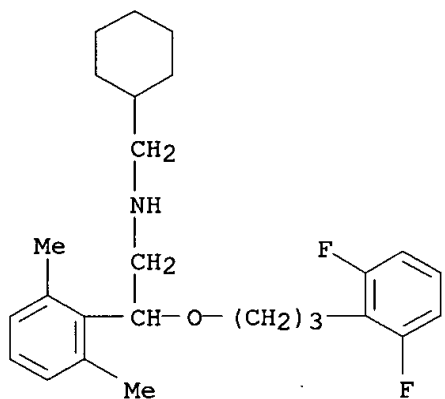
RN 401938-51-0 CAPLUS

CN Benzeneethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-N,N-diethyl-2,6-dimethyl- (9CI) (CA INDEX NAME)



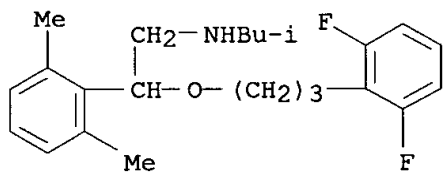
RN 401938-53-2 CAPLUS

CN Benzenethanamine, N-(cyclohexylmethyl)-.beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl- (9CI) (CA INDEX NAME)



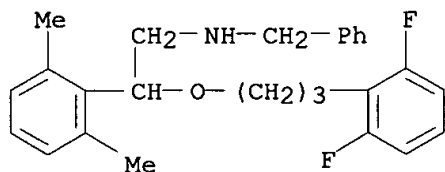
RN 401938-55-4 CAPLUS

CN Benzenethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)



RN 401938-57-6 CAPLUS

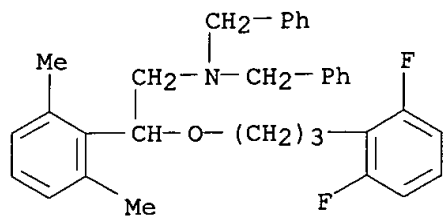
CN Benzenethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 401938-59-8 CAPLUS

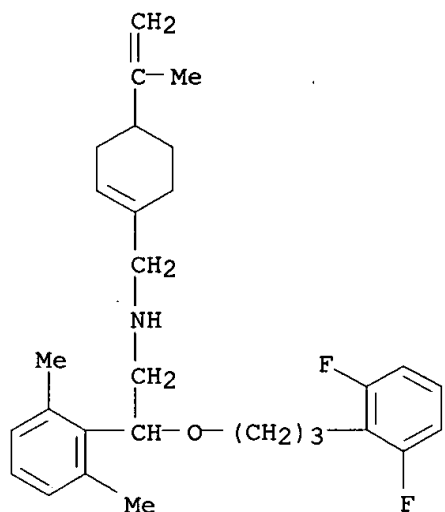
CN Benzenethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl-N,N-diphenyl- (9CI) (CA INDEX NAME)

bis(phenylmethyl)- (9CI) (CA INDEX NAME)



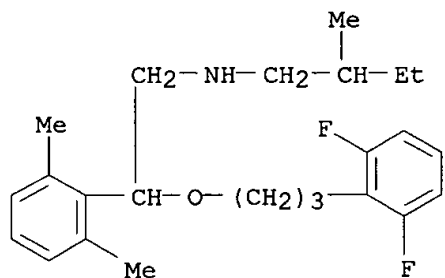
RN 401938-61-2 CAPLUS

CN Benzenethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl-N-[[4-(1-methylethenyl)-1-cyclohexen-1-yl]methyl]- (9CI) (CA INDEX NAME)



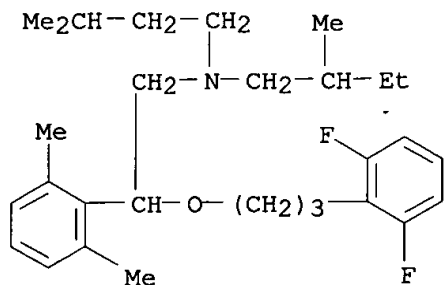
RN 401938-63-4 CAPLUS

CN Benzenethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl-N-(2-methylbutyl)- (9CI) (CA INDEX NAME)



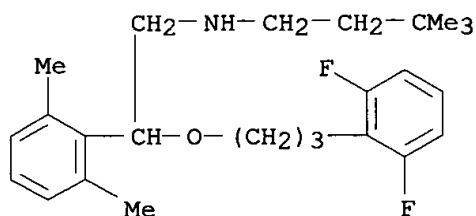
RN 401938-67-8 CAPLUS

CN Benzenethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl-N-(2-methylbutyl)-N-(3-methylbutyl)- (9CI) (CA INDEX NAME)



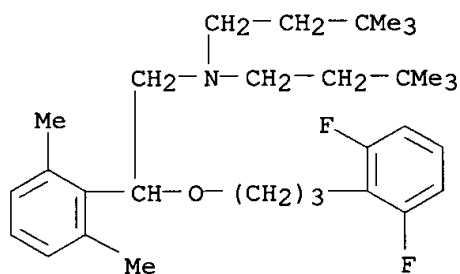
RN 401938-69-0 CAPLUS

CN Benzeneethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-N-(3,3-dimethylbutyl)-2,6-dimethyl- (9CI) (CA INDEX NAME)



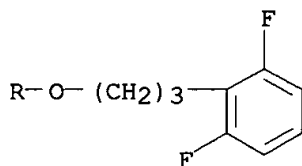
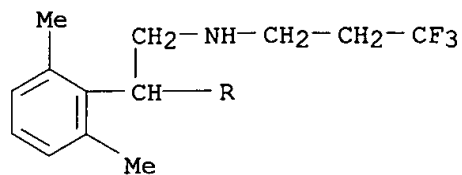
RN 401938-71-4 CAPLUS

CN Benzeneethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-N,N-bis(3,3-dimethylbutyl)-2,6-dimethyl- (9CI) (CA INDEX NAME)



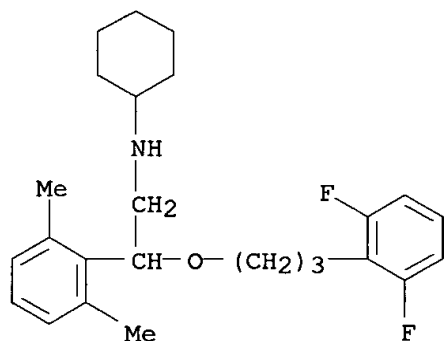
RN 401938-73-6 CAPLUS

CN Benzeneethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl-N-(3,3,3-trifluoropropyl)- (9CI) (CA INDEX NAME)



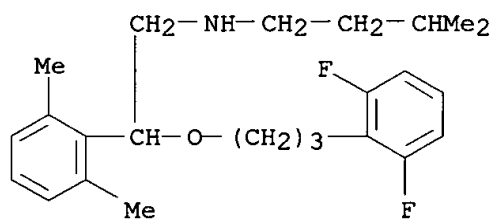
RN 401938-75-8 CAPLUS

CN Benzeneethanamine, N-cyclohexyl-.beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl- (9CI) (CA INDEX NAME)



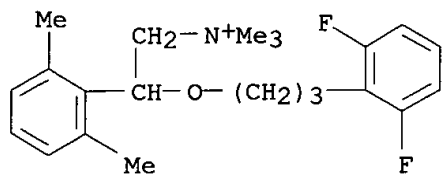
RN 401938-77-0 CAPLUS

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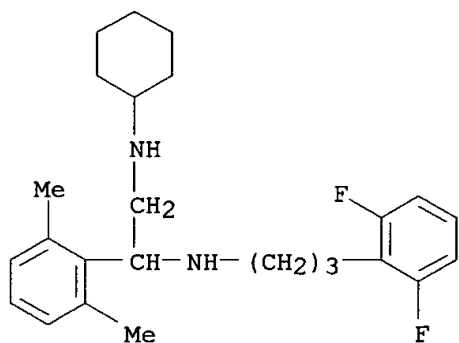
RN 401938-79-2 CAPLUS

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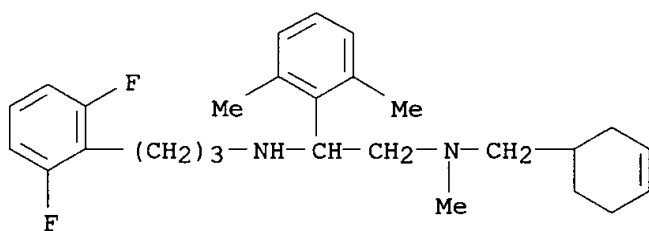
RN 401939-43-3 CAPLUS

CN 1,2-Ethanediamine, N2-cyclohexyl-N1-[3-(2,6-difluorophenyl)propyl]-1-(2,6-dimethylphenyl)- (9CI) (CA INDEX NAME)



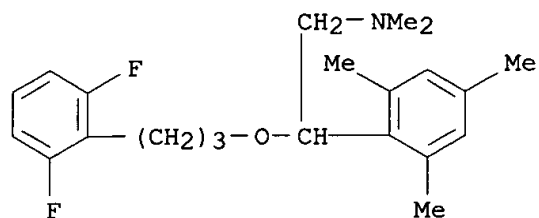
RN 401939-45-5 CAPLUS

CN 1,2-Ethanediamine, N2-(3-cyclohexen-1-ylmethyl)-N1-[3-(2,6-difluorophenyl)propyl]-1-(2,6-dimethylphenyl)-N2-methyl- (9CI) (CA INDEX NAME)

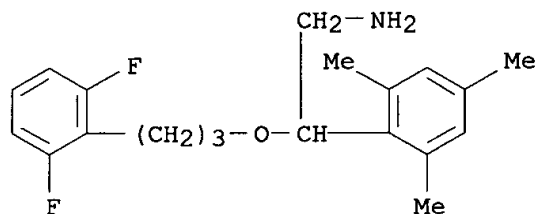


RN 401939-49-9 CAPLUS

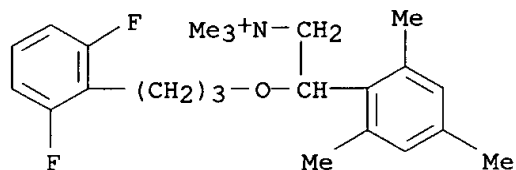
CN Benzeneethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-N,N,2,4,6-pentamethyl- (9CI) (CA INDEX NAME)



RN 401939-51-3 CAPLUS

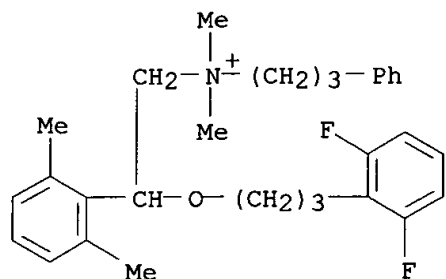
CN Benzeneethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-2,4,6-trimethyl-  
(9CI) (CA INDEX NAME)

RN 401939-53-5 CAPLUS

CN Benzeneethanaminium, .beta.-[3-(2,6-difluorophenyl)propoxy]-N,N,N,2,4,6-  
hexamethyl-, iodide (9CI) (CA INDEX NAME)● I<sup>-</sup>

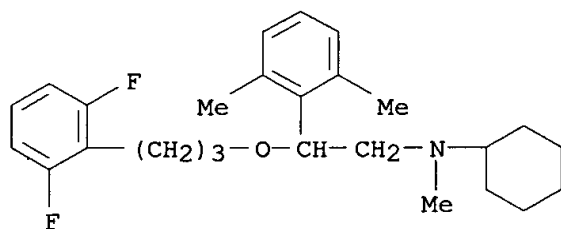
RN 401939-54-6 CAPLUS

CN Benzenepropanaminium, N-[2-[3-(2,6-difluorophenyl)propoxy]-2-(2,6-  
dimethylphenyl)ethyl]-N,N-dimethyl-, iodide (9CI) (CA INDEX NAME)

● I<sup>-</sup>

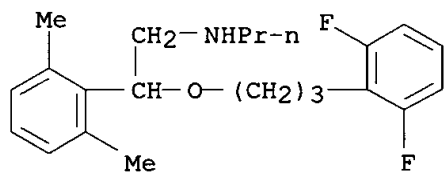
RN 401939-55-7 CAPLUS

CN Benzeneethanamine, N-cyclohexyl-.beta.-[3-(2,6-difluorophenyl)propoxy]-N,2,6-trimethyl- (9CI) (CA INDEX NAME)



RN 401939-56-8 CAPLUS

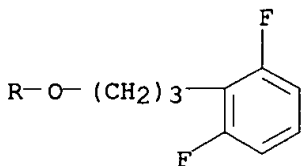
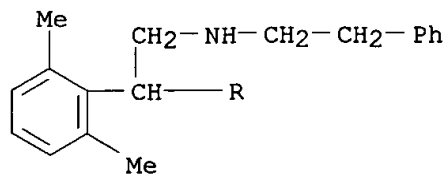
CN Benzeneethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl-N-propyl- (9CI) (CA INDEX NAME)



RN 401939-58-0 CAPLUS

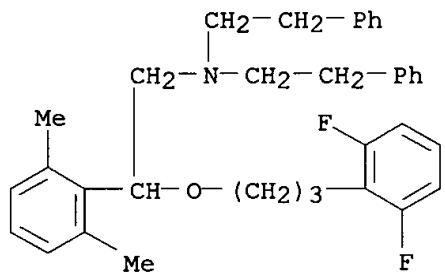
CN Benzeneethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl-N-(2-phenylethyl)- (9CI) (CA INDEX NAME)





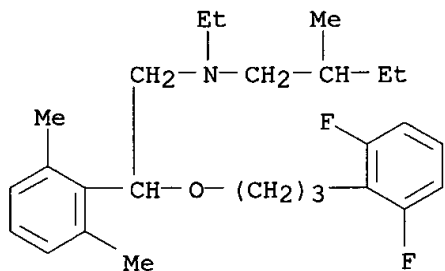
RN 401939-60-4 CAPLUS

CN Benzeneethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl-N,N-bis(2-phenylethyl)- (9CI) (CA INDEX NAME)



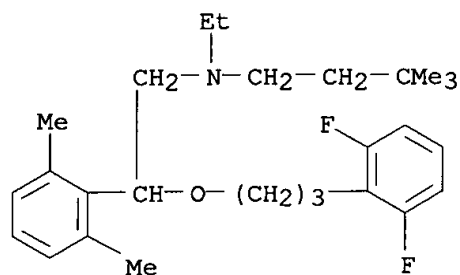
RN 401939-62-6 CAPLUS

CN Benzeneethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-N-ethyl-2,6-dimethyl-N-(2-methylbutyl)- (9CI) (CA INDEX NAME)



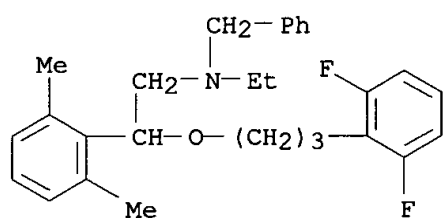
RN 401939-64-8 CAPLUS

CN Benzeneethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-N-(3,3-dimethylbutyl)-N-ethyl-2,6-dimethyl- (9CI) (CA INDEX NAME)



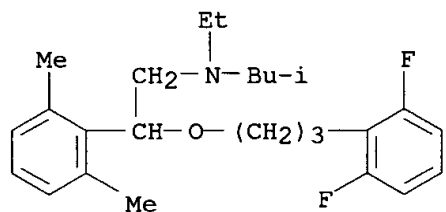
RN 401939-66-0 CAPLUS

CN Benzenethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-N-ethyl-2,6-dimethyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



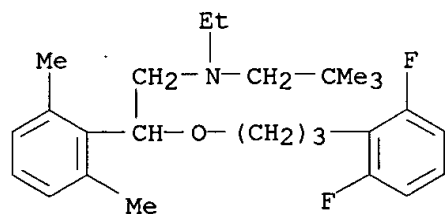
RN 401939-68-2 CAPLUS

CN Benzenethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-N-ethyl-2,6-dimethyl-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)



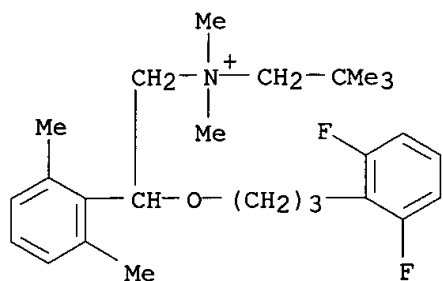
RN 401939-70-6 CAPLUS

CN Benzenethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-N-(2,2-dimethylpropyl)-N-ethyl-2,6-dimethyl- (9CI) (CA INDEX NAME)



RN 401939-72-8 CAPLUS

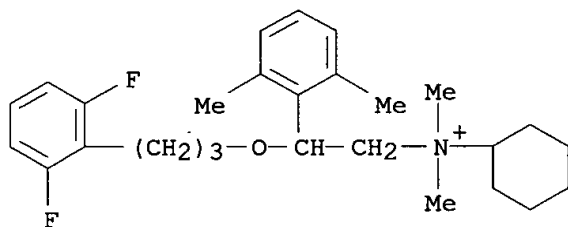
CN Benzenethanaminium, .beta.-[3-(2,6-difluorophenyl)propoxy]-N-(2,2-dimethylpropyl)-N,N,2,6-tetramethyl-, iodide (9CI) (CA INDEX NAME)



● I<sup>-</sup>

RN 401939-74-0 CAPLUS

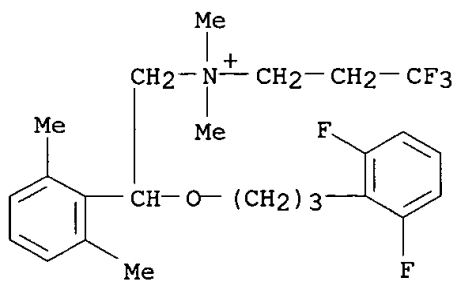
CN Benzenethanaminium, N-cyclohexyl-.beta.-[3-(2,6-difluorophenyl)propoxy]-N,N,2,6-tetramethyl-, iodide (9CI) (CA INDEX NAME)



● I<sup>-</sup>

RN 401939-76-2 CAPLUS

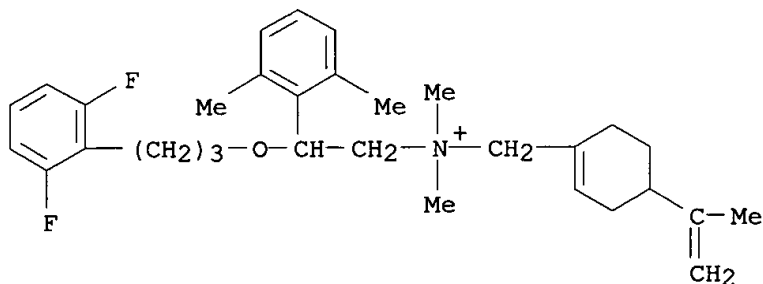
CN Benzenethanaminium, .beta.-[3-(2,6-difluorophenyl)propoxy]-N,N,2,6-tetramethyl-N-(3,3,3-trifluoropropyl)-, iodide (9CI) (CA INDEX NAME)



I<sup>-</sup>

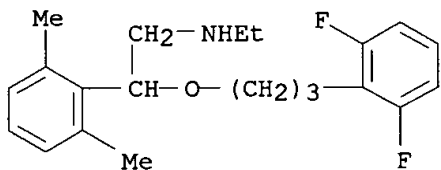
RN 401939-78-4 CAPLUS

CN Benzeneethanaminium, .beta.-[3-(2,6-difluorophenyl)propoxy]-N,N,2,6-tetramethyl-N-[[4-(1-methylethenyl)-1-cyclohexen-1-yl]methyl]-, iodide (9CI) (CA INDEX NAME)

● I<sup>-</sup>

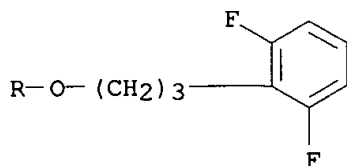
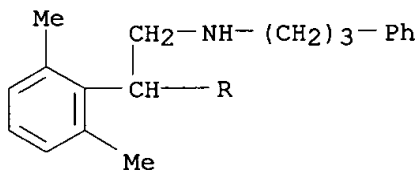
RN 401939-80-8 CAPLUS

CN Benzeneethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-N-ethyl-2,6-dimethyl- (9CI) (CA INDEX NAME)



RN 401939-82-0 CAPLUS

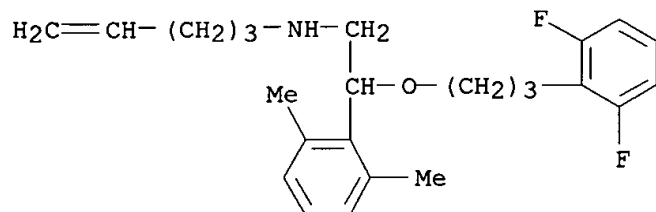
CN Benzenepropanamine, N-[2-[3-(2,6-difluorophenyl)propoxy]-2-(2,6-dimethylphenyl)ethyl]- (9CI) (CA INDEX NAME)



RN 401939-84-2 CAPLUS

CN Benzeneethanamine, .beta.-[3-(2,6-difluorophenyl)propoxy]-2,6-dimethyl-N-4-

pentenyl- (9CI) (CA INDEX NAME)

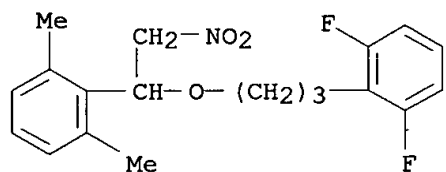


IT 401940-02-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. of phenylethanamines and phenylalkylethanamines as sodium channel blockers)

RN 401940-02-1 CAPLUS

CN Benzene, 2-[1-[3-(2,6-difluorophenyl)propoxy]-2-nitroethyl]-1,3-dimethyl- (9CI) (CA INDEX NAME)

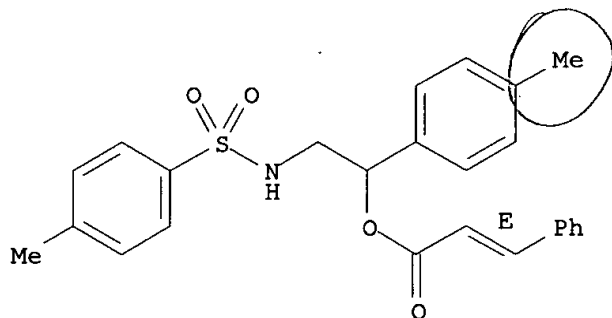


RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

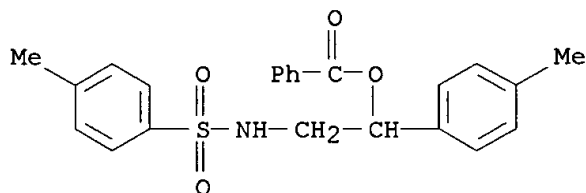
L6 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2003 ACS  
 AN 2002:149710 CAPLUS  
 DN 137:154696  
 TI Indium triflate-catalyzed ring opening of aziridines with carboxylic acids  
 AU Yadav, J. S.; Subba Reddy, B. V.; Sadashiv, K.; Harikishan, K.  
 CS Division of Organic Chemistry, Indian Institute of Chemical Technology,  
 Hyderabad, 500007, India  
 SO Tetrahedron Letters (2002), 43(11), 2099-2101  
 CODEN: TELEAY; ISSN: 0040-4039  
 PB Elsevier Science Ltd.  
 DT Journal  
 LA English  
 OS CASREACT 137:154696  
 AB Aziridines, e.g. I, react smoothly with carboxylic acids, e.g. acetic  
 acid, in the presence of a catalytic amt. of indium triflate at ambient  
 temp. to afford the corresponding .beta.-amino acetates and benzoates in  
 high yields with high regioselectivity.  
 IT **445425-59-2P 445425-61-6P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (indium triflate-catalyzed regio- and stereoselective ring opening of  
 aziridines with carboxylic acids)  
 RN 445425-59-2 CAPLUS  
 CN 2-Propenoic acid, 3-phenyl-, 1-(4-methylphenyl)-2-[[4-  
 methylphenyl)sulfonyl]amino]ethyl ester, (2E)- (9CI) (CA INDEX NAME)

*not find*

Double bond geometry as shown.



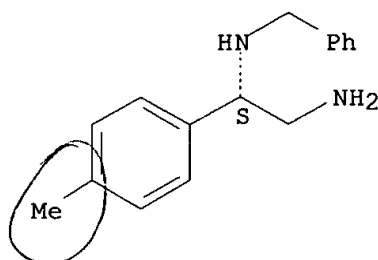
RN 445425-61-6 CAPLUS  
 CN Benzenesulfonamide, N-[2-(benzoyloxy)-2-(4-methylphenyl)ethyl]-4-methyl-  
 (9CI) (CA INDEX NAME)



RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

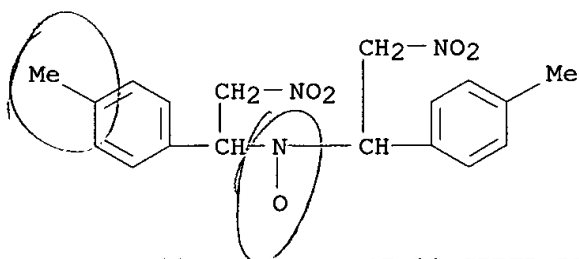
L6 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2003 ACS  
 AN 1998:715815 CAPLUS  
 DN 130:153215  
 TI Syntheses of optically active .alpha.-amino nitriles by asymmetric transformation of the second kind using a principle of O. Dimroth  
 AU Hassan, Nasser A.; Bayer, Erwin; Jochims, Johannes C.  
 CS Fakultat fur Chemie, Universitat Konstanz, Konstanz, D-78434, Germany  
 SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1998), (22), 3747-3758  
 CODEN: JCPRB4; ISSN: 0300-922X  
 PB Royal Society of Chemistry  
 DT Journal  
 LA English  
 AB A mixt. of solids As and Bs in equil. with the dissolved compds. A1 and B1 is transformed completely into one pure solid, say Bs, if the dissolved compds. A1.rdblhar.eB1 are equilibrating in soln. This principle is applied to transform 1:1 mixts. of solid diastereomeric amygdalates (R,R)-I+(S,R)-I, prepd. from racemic .alpha.-amino nitriles (R,S)-II with (R)-mandelic acid into stereochem. pure single diastereomers (R,R)-I, or (S,R)-I (de > 97%) (asym. transformation of the second kind by application of Dimroth's principle). Decompn. of the amygdalates (R,R)-I, or (S,R)-I, with aq. base affords the enantiomerically pure .alpha.-amino nitriles (R)-II, or (S)-II. The chiral auxiliary (R)-mandelic acid is recovered almost quant. The optically active .alpha.-amino nitriles are hydrolyzed to amides or further to .alpha.-N-alkylamino acids. N-Benzylamino acids are hydrogenated to .alpha.-amino acids. Some of the optically active .alpha.-amino nitriles II are reduced to optically active 1,2-diamines. In most cases, abs. configurations could be assigned by comparison of the sp. rotations obsd. with those of authentic compds.  
 IT **220131-03-3P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of optically active amino acids and diamines via kinetic resolu. of .alpha.-amino nitriles)  
 RN 220131-03-3 CAPLUS  
 CN 1,2-Ethanediamine, 1-(4-methylphenyl)-N1-(phenylmethyl)-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RE.CNT 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2003 ACS  
 AN 1998:367425 CAPLUS  
 DN 129:135789  
 TI Photochemical nitration by tetranitromethane. Part XLIII. Photolysis of some styrene derivatives with tetranitromethane: mechanism of isoxazolidine formation  
 AU Eberson, Lennart; Hartshorn, Michael P.; Persson, Ola  
 CS Department of Chemistry, Lund University, Lund, S-221 00, Swed.  
 SO Acta Chemica Scandinavica (1998), 52(6), 751-760  
 CODEN: ACHSE7; ISSN: 0904-213X  
 PB Munksgaard International Publishers Ltd.  
 DT Journal  
 LA English  
 OS CASREACT 129:135789  
 AB The photochem. reaction of tetranitromethane in dichloromethane or acetonitrile with 4-methylstyrene, styrene, 4-chlorostyrene, 3-chlorostyrene or 4-acetoxystyrene gives two stereoisomeric isoxazolidines, 2-(2'-nitro-1'-X-phenyl)ethoxy-3,3-dinitro-5-(X-phenyl)isoxazolidines, a nitro ketone, nitromethyl ketone, and a nitronic ester, 3-nitro-5-(X-phenyl)-2-isoxazoline N-oxide. In each case, the (RS,RS)-stereoisomer is the major isoxazolidine formed. The first step of the reaction is the photogeneration of the triad [2.cntdot.+ NO<sub>2</sub> (NO<sub>2</sub>)<sub>3</sub>C-]. In the formation of isoxazolidines, and of the nitronic esters, the key intermediate is assumed to be the substituted aminoxyl, 3,3-dinitro-4-(X-phenyl)isoxazolidin-N-oxyl radical formed by reaction of the substituted styrene radical cation (2.cntdot.+) with trinitromethanide ion followed by cyclization of a resulting carbon radical.  
 IT **210537-21-6P**  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (photolysis of styrene derivs. with tetranitromethane and mechanism of isoxazolidine formation)  
 RN 210537-21-6 CAPLUS  
 CN Nitroxide, bis[1-(4-methylphenyl)-2-nitroethyl] (9CI) (CA INDEX NAME)



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT



L6 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2003 ACS

AN 1996:487416 CAPLUS

DN 125:247685

TI A solid-phase synthesis of miconazole analogs via an iodoetherification reaction

AU Tortolani, David R.; Biller, Scott A.

CS Bristol-Myers Squibb Pharm. Res. Inst., Princeton, NJ, 08543, USA

SO Tetrahedron Letters (1996), 37(32), 5687-5690

CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier

DT Journal

LA English

AB A procedure for the prepn. of various analogs of miconazole, I and II (R = 2,4,6-Me<sub>3</sub>, 3,5-F<sub>2</sub>, 4-cyclohexylphenyl, 3-Br, etc.), on solid support is described. A novel iodoetherification transformation is utilized as the key synthetic step. Thus, treatment of 4-(HOCH<sub>2</sub>)C<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>CH<sub>2</sub>-X (X = polymer resin) with 2,4,6-Me<sub>3</sub>C<sub>6</sub>H<sub>2</sub>CH:CH<sub>2</sub> and N-iodosuccinimide in the presence of triflic acid gave the iodoethyl ether 2,4,6-Me<sub>3</sub>C<sub>6</sub>H<sub>2</sub>CH(CH<sub>2</sub>I)OCH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>CH<sub>2</sub>-X, while underwent substitution reaction with (trimethylsilyl)imidazole and then resin cleavage to give I (R = 2,4,6-Me<sub>3</sub>). This approach has been applied to the combinatorial synthesis of 45 analogs.

IT 182132-35-0P 182132-44-1P 182132-46-3P

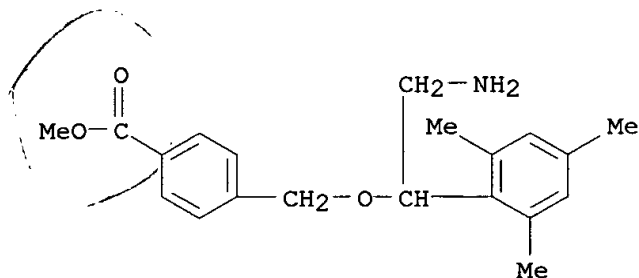
182132-53-2P 182132-54-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(solid-phase synthesis of miconazole analogs via iodoetherification)

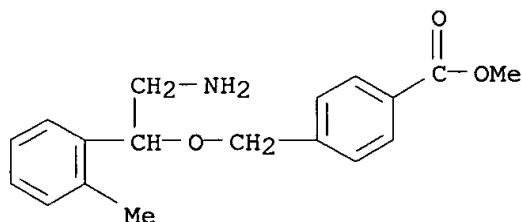
RN 182132-35-0 CAPLUS

CN Benzoic acid, 4-[[2-amino-1-(2,4,6-trimethylphenyl)ethoxy]methyl]-, methyl ester (9CI) (CA INDEX NAME)



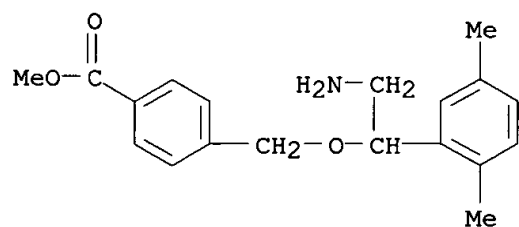
RN 182132-44-1 CAPLUS

CN Benzoic acid, 4-[[2-amino-1-(2-methylphenyl)ethoxy]methyl]-, methyl ester (9CI) (CA INDEX NAME)



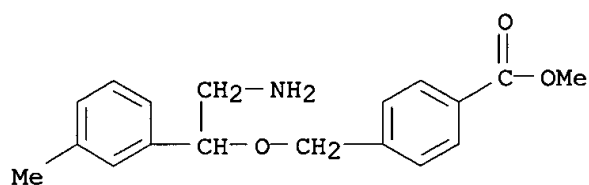
RN 182132-46-3 CAPLUS

CN Benzoic acid, 4-[[2-amino-1-(2,5-dimethylphenyl)ethoxy]methyl]-, methyl ester (9CI) (CA INDEX NAME)



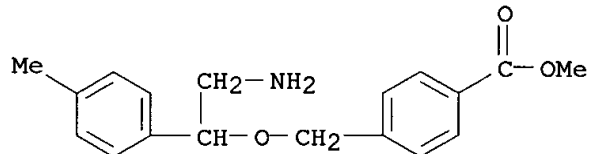
RN 182132-53-2 CAPLUS

CN Benzoic acid, 4-[[2-amino-1-(3-methylphenyl)ethoxy]methyl]-, methyl ester  
(9CI) (CA INDEX NAME)

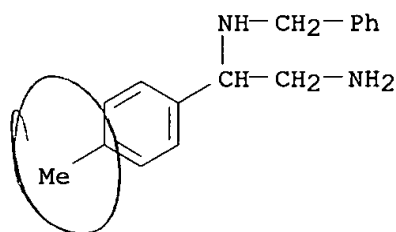


RN 182132-54-3 CAPLUS

CN Benzoic acid, 4-[[2-amino-1-(4-methylphenyl)ethoxy]methyl]-, methyl ester  
(9CI) (CA INDEX NAME)

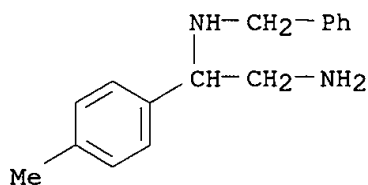


L6 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2003 ACS  
 AN 1990:458588 CAPLUS  
 DN 113:58588  
 TI Adrenergic agents. II. 1-Aryl-N2-alkylethanediamines as isosters of adrenergic arylethanolamines  
 AU Berger, Sarah; Nudelman, Abraham  
 CS Chem. Dep., Bar Ilan Univ., Ramat Gan, 52900, Israel  
 SO Archiv der Pharmazie (Weinheim, Germany) (1990), 323(4), 229-33  
 CODEN: ARPMAS; ISSN: 0365-6233  
 DT Journal  
 LA English  
 OS CASREACT 113:58588  
 AB A family of 1-aryl-N2-alkylethanediamines  $\text{ArCH}(\text{NHR})\text{CH}_2\text{NH}_2$  (I, Ar = substituted Ph, naphthyl, furyl, R = H) isosteric with the N-alkylarylethanolamines are described. Although the prepd. compds. were generally less potent than the N-alkylarylethanolamines, the 1-aryl-N'-(phenylmethyl)-N-alkyl-1,2-ethanediamine derivs. I (R =  $\text{CH}_2\text{Ph}$ ), are more active than the debenzylated free amino analogs, which may be indicative of the importance of the lipophilicity of the substituent at the .alpha. position to the arom. ring.  
 IT **40658-72-8P 110618-88-7P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. and isopropylation of)  
 RN 40658-72-8 CAPLUS  
 CN 1,2-Ethanediamine, 1-(4-methylphenyl)-N1-(phenylmethyl)-, dihydrochloride (9CI) (CA INDEX NAME)



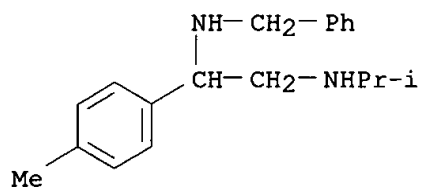
● 2 HCl

RN 110618-88-7 CAPLUS  
 CN 1,2-Ethanediamine, 1-(4-methylphenyl)-N1-(phenylmethyl)- (9CI) (CA INDEX NAME)



IT **128349-20-2P 128349-27-9P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn., adrenergic activity, and debenzylation of)  
 RN 128349-20-2 CAPLUS

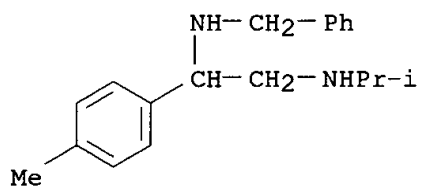
CN 1,2-Ethanediamine, N2-(1-methylethyl)-1-(4-methylphenyl)-N1-(phenylmethyl)-  
, dihydrochloride (9CI) (CA INDEX NAME)



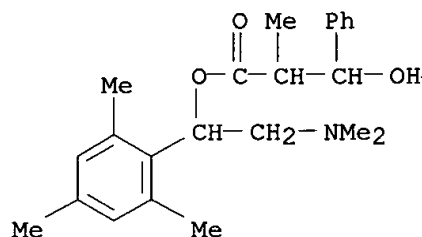
●2 HCl

RN 128349-27-9 CAPLUS

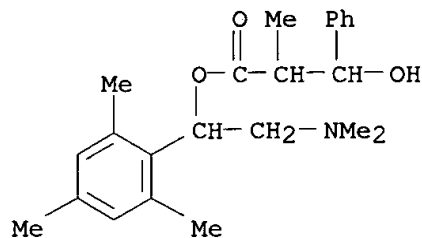
CN 1,2-Ethanediamine, N2-(1-methylethyl)-1-(4-methylphenyl)-N1-(phenylmethyl)-  
(9CI) (CA INDEX NAME)



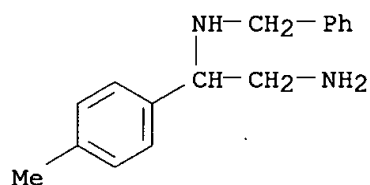
L6 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2003 ACS  
 AN 1990:440077 CAPLUS  
 DN 113:40077  
 TI Auxiliary structure and asymmetric induction in the Mukaiyama-aldol reactions of chiral silyl ketene acetals  
 AU Gennari, Cesare; Molinari, Francesco; Cozzi, PierGiorgio; Oliva, Ambrogio  
 CS Dip. Chim. Org. Ind. Nat., Univ. Milano, Milan, 20133, Italy  
 SO Tetrahedron Letters (1989), 30(38), 5163-6  
 CODEN: TELEAY; ISSN: 0040-4039  
 DT Journal  
 LA English  
 OS CASREACT 113:40077  
 AB A variety of chiral auxiliaries [e.g., (1S,2R-Me<sub>2</sub>NCHMeCHPhOH, (S)-Me<sub>2</sub>NCH<sub>2</sub>CHMeOH] were prepd. and tested for levels of asym. induction control in the Mukaiyama-aldol reaction of chiral silyl ketene acetals. Structural features required for high levels of control are discussed.  
 IT **127677-18-3P 127759-16-4P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)  
 RN 127677-18-3 CAPLUS  
 CN Benzenepropanoic acid, .beta.-hydroxy-.alpha.-methyl-, 2-(dimethylamino)-1-(2,4,6-trimethylphenyl)ethyl ester, [.alpha.R-[.alpha.R\*(S\*),.beta.S\*]]- (9CI) (CA INDEX NAME)



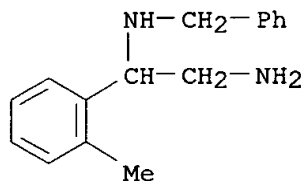
RN 127759-16-4 CAPLUS  
 CN Benzenepropanoic acid, .beta.-hydroxy-.alpha.-methyl-, 2-(dimethylamino)-1-(2,4,6-trimethylphenyl)ethyl ester, [.alpha.R-[.alpha.R\*(S\*),.beta.R\*]]- (9CI) (CA INDEX NAME)



L6 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2003 ACS  
 AN 1987:554281 CAPLUS  
 DN 107:154281  
 TI Derivatives of 5-phenylimidazolidin-2-one  
 AU Tkaczynski, Tadeusz; Tkaczynska, Danuta  
 CS Dep. Chem. Technol. Pharm. Prod., Sch. Med., Lublin, 20-081, Pol.  
 SO Acta Poloniae Pharmaceutica (1986), 43(4), 319-21  
 CODEN: APPHAX; ISSN: 0001-6837  
 DT Journal  
 LA Polish  
 OS CASREACT 107:154281  
 AB Ten title derivs. I (R = H, R1 = Et, Pr, Bu, Me2CHCH2; R = 2-Cl, R1 = Me, Me2CHCH2, PhCH2; R = 4-Cl, R1 = Me; R = 4-Me, R1 = Me, PhCH2) were prepd. in 40-78% yields by heating the corresponding RC6H4CH(NHR1)CH2NH2 (R and R1 as above) with urea.  
 IT **110618-88-7**  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with urea, imidazolidinone deriv. from)  
 RN 110618-88-7 CAPLUS  
 CN 1,2-Ethanediamine, 1-(4-methylphenyl)-N1-(phenylmethyl)- (9CI) (CA INDEX NAME)

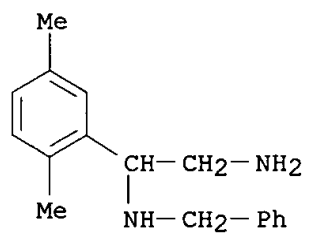


L6 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2003 ACS  
 AN 1984:174724 CAPLUS  
 DN 100:174724  
 TI Synthesis and central nervous system properties of 2-  
 [(alkoxycarbonyl)amino]-4(5)-phenyl-2-imidazolines  
 AU Weinhardt, Klaus; Beard, Colin C.; Dvorak, Charles; Marx, Michael;  
 Patterson, John; Roszkowski, Adolph; Schuler, Margery; Unger, Stefan H.;  
 Wagner, Paul J.; Wallach, Marshall B.  
 CS Inst. Org. Chem., Syntex Res., Palo Alto, CA, 94304, USA  
 SO Journal of Medicinal Chemistry (1984), 27(5), 616-27  
 CODEN: JMCMAR; ISSN: 0022-2623  
 DT Journal  
 LA English  
 AB The title compds. e.g. I [R = (un)substituted Ph, R1 = H, alkyl; R2 =  
 alkoxycarbonyl, R3 = H, Me; RR3 = o-C6H4CH2) were prepd. from 1,2-diamines  
 and MeSC(:NR2)NHR2. I were evaluated for central nervous system (CNS)  
 effects (antidepressant, anticonvulsant, muscle relaxant, and depressant)  
 in animal models. Some sepn. of those CNS activities was achieved through  
 substitutions on the Ph and imidazoline moieties. Halo-substituted Ph  
 compds. were among the most potent antidepressants, while imidazoline  
 N-alkylation produced compds. with increased depressant effects (loss of  
 righting reflex, mouse behavior). Comparison of in vitro and in vivo data  
 for pairs of 2-[(methoxycarbonyl)amino]-4(5)-phenyl-2-imidazolines and  
 their parent 2-amino-4(5)-phenyl-2-imidazolines, suggests that I were  
 prodrugs for the latter in inhibition of norepinephrine reuptake.  
 IT **89145-86-8P 89145-99-3P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and cyclocondensation with bis(alkoxycarbonyl) derivs. of  
 methylthiopseudourea, imidazoline deriv. from)  
 RN 89145-86-8 CAPLUS  
 CN 1,2-Ethanediamine, 1-(2-methylphenyl)-N1-(phenylmethyl)-, dihydrochloride  
 (9CI) (CA INDEX NAME)



●2 HCl

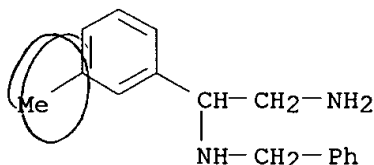
RN 89145-99-3 CAPLUS  
 CN 1,2-Ethanediamine, 1-(2,5-dimethylphenyl)-N1-(phenylmethyl)-,  
 dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl



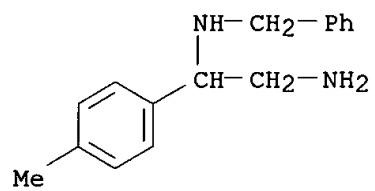
L6 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2003 ACS  
 AN 1974:10249 CAPLUS  
 DN 80:10249  
 TI Antihypertensive agents. Synthesis and biological properties of  
 2-amino-4-aryl-2-imidazolines  
 AU Matier, W. L.; Owens, D. A.; Comer, W. T.; Deitchman, D.; Ferguson, H. C.;  
 Seidehamel, R. J.; Young, J. R.  
 CS Dep. Chem. Res., Mead Johnson Res. Cent., Evansville, IN, USA  
 SO Journal of Medicinal Chemistry (1973), 16(8), 901-8  
 CODEN: JMCMAR; ISSN: 0022-2623  
 DT Journal  
 LA English  
 AB The antihypertensive activity of 2-amino-4-aryl-2-imidazolines showed no  
 close correlation with peripheral neuronal norepinephrine [51-41-2] uptake  
 or release (mouse heart in vivo), sympathetic neuronal blocking activity  
 (rabbit jejunum in vitro), or prevention of reserpine-induced ptosis in  
 mice. Greatest antihypertensive activity was shown by  
 2-amino-4-(3,4-dichlorophenyl)-2-imidazoline-HBr (I) [43026-98-8] (5 mg/kg  
 s.c. in DOCA-hypertensive rats); I was also active orally in  
 DOCA-hypertensive and spontaneously hypertensive rats and was more potent  
 than guanethidine or bethanidine. I was also the most potent inhibitor of  
 norepinephrine release and uptake and moderately active as a neuronal  
 blocker. 4-(2-Chlorophenyl)-2-hydrazino-2-imidazoline-HI [43026-99-9] and  
 2-benzylidenehydrazino-4-(2-chlorophenyl)-2-imidazoline-HI [43027-00-5]  
 were the most potent neuronal blockers in the series, being 10 times as  
 potent as bethanidine, and were among the most potent stimulants of  
 norepinephrine release and moderately active as antihypertensive agents.  
 I was prepd. by cyclizing the appropriate .beta.-aminophenylethylamine  
 with BrCN.  
 IT **40658-71-7P 40658-72-8P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)  
 RN 40658-71-7 CAPLUS  
 CN 1,2-Ethanediamine, 1-(3-methylphenyl)-N1-(phenylmethyl)-, dihydrochloride  
 (9CI) (CA INDEX NAME)



\* 2 second ethz  
 \* ethz position different.

● 2 HCl

RN 40658-72-8 CAPLUS  
 CN 1,2-Ethanediamine, 1-(4-methylphenyl)-N1-(phenylmethyl)-, dihydrochloride  
 (9CI) (CA INDEX NAME)



● 2 HCl

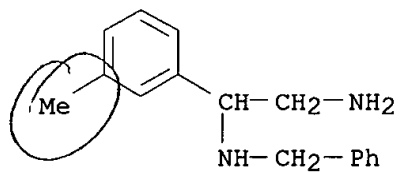
L6 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2003 ACS  
 AN 1973:136297 CAPLUS  
 DN 78:136297  
 TI Neuron blocking antihypertensive 2-amino-4-phenyl-2-imidazoline salts  
 IN Matier, William Lesley; Comer, William Timmey  
 PA Bristol-Myers Co.  
 SO Ger. Offen., 68 pp.  
 CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

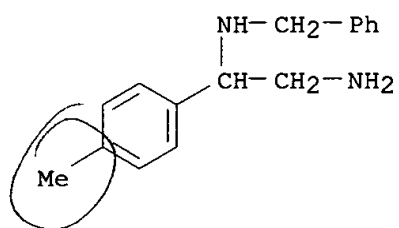
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	CA 1018174	A1	19770927	CA 1972-148323	19720731
	FR 2150766	A1	19730413	FR 1972-29037	19720811
	ZA 7205522	A	19730425	ZA 1972-5522	19720811
	GB 1347930	A	19740227	GB 1972-37488	19720811
	IL 40123	A1	19750522	IL 1972-40123	19720814
	AU 7245593	A1	19740221	AU 1972-45593	19720815
	HU 165660	P	19741028	HU 1972-BI451	19720815
	CH 579055	A	19760831	CH 1972-12081	19720815
	CH 591451	A	19770915	CH 1975-13579	19720815
	DK 139098	C	19790528	DK 1972-4039	19720815
	DK 139098	B	19781218		
	SE 406763	C	19790607	SE 1972-10578	19720815
	SE 406763	B	19790226		
	BE 787617	A1	19730216	BE 1972-121019	19720816
	NL 7211173	A	19730220	NL 1972-11173	19720816
	JP 48029770	A2	19730419	JP 1972-81545	19720816
	JP 57019106	B4	19820420		
	US 3898342	A	19750805	US 1974-477718	19740610
PRAI	US 1971-172321		19710816		
	US 1972-268380		19720703		
AB	About forty title salts [I, Rn = Cl, Me, 4-CF <sub>3</sub> , 2,4-Cl <sub>2</sub> , 2,6-Cl <sub>2</sub> , 4-MeO, 4-PhCH <sub>2</sub> O; R1 = H, Me, NHOH, N:CM <sub>2</sub> , (CH <sub>2</sub> ) <sub>3</sub> NMe <sub>2</sub> , Bz, CH <sub>2</sub> Ph, N:CHPh; R2 = H, PhCH <sub>2</sub> ; X = Cl, Br, iodide, 0.5 fumarate] were prepd. and used as neuron blockers and antihypertensives. Thus, treatment of o-ClC <sub>6</sub> H <sub>4</sub> CHO with NaCN and PhCH <sub>2</sub> NH <sub>2</sub> .HCl for 5 hr in aq. MeOH gave PhCH <sub>2</sub> NHCH(CN)C <sub>6</sub> H <sub>4</sub> Cl-o.HCl (II). Similarly prepd. were .apprx.20 other aminophenylacetonitriles. The free base of II was reduced with LiAlH <sub>4</sub> in Et <sub>2</sub> O under N and HCl added to give 97% PhCH <sub>2</sub> NHCH(CH <sub>2</sub> NH <sub>2</sub> )C <sub>6</sub> H <sub>4</sub> Cl-o.HCl (III). Similarly prepd. were .apprx.20 other 1-phenylethylenediamines. Hydrogenation of III over Pd/C in MeOH gave o-ClC <sub>6</sub> H <sub>4</sub> CH(NH <sub>3</sub> NH <sub>2</sub> .2HCl (IV)). Treatment of the free base of IV with BrCN in benzene for 4 hr at room temp. gave I (Rn = o-Cl, R1 = R2 = H, X = Br).				
IT	<b>40658-71-7P 40658-72-8P</b>				
	RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)				
RN	40658-71-7 CAPLUS				
CN	1,2-Ethanediamine, 1-(3-methylphenyl)-N1-(phenylmethyl)-, dihydrochloride (9CI) (CA INDEX NAME)				



●2 HCl

RN 40658-72-8 CAPLUS

CN 1,2-Ethanediamine, 1-(4-methylphenyl)-N1-(phenylmethyl)-, dihydrochloride  
(9CI) (CA INDEX NAME)



●2 HCl

L6 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2003 ACS

AN 1972:3004 CAPLUS

DN 76:3004

TI Electron spin resonance study of nitroxides formed in the reaction of nitrogen dioxide and nitrogen oxide with styrenes

AU Jonkman, Leffert; Muller, Hans; Kommandeur, Jan

CS Lab. Phys. Chem., Univ. Groningen, Groningen, Neth.

SO Journal of the American Chemical Society (1971), 93(22), 5833-8

CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

AB When NO<sub>2</sub> reacts with styrenes ACR:CH<sub>2</sub> (A = Ph, 2,4,6-Me<sub>3</sub>C<sub>6</sub>H<sub>2</sub>; R = H, Me) in the presence of nitrosobenzene, phenyl(1-aryl-2-nitroethyl) nitroxides ACR(CH<sub>2</sub>NO<sub>2</sub>)N(O)Ph are formed through the reaction of .beta.-nitroalkyl radicals .bul.CARCH<sub>2</sub>NO<sub>2</sub> (I) with nitrosobenzene. In the reaction of NO<sub>2</sub>-NO mixts. with styrenes, bis(1-aryl-2-nitroethyl) nitroxides ON(CARCH<sub>2</sub>NO<sub>2</sub>)<sub>2</sub> (II) are formed by the reaction of I with the .alpha.-nitroso-.beta.-nitro addn. products ACR(NO)CH<sub>2</sub>NO<sub>2</sub> (III) of the styrenes. Both diastereomers of II (meso, and d,l) were observed with all styrenes investigated, except for those with ortho substituents. Dissocn. of the dimer of III is accompanied by decompn. of III into NO and the radical I with subsequent formation of the nitroxide II.

IT 34817-97-5 34940-04-0

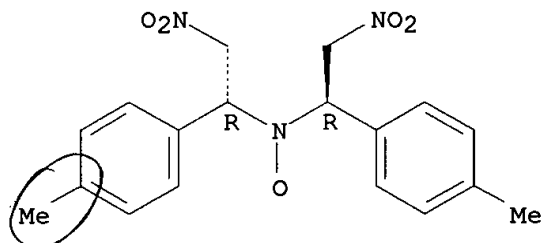
RL: PRP (Properties)

(E.S.R. of)

RN 34817-97-5 CAPLUS

CN Nitroxide, bis[1-(4-methylphenyl)-2-nitroethyl], (R\*,R\*)- (9CI) (CA INDEX NAME)

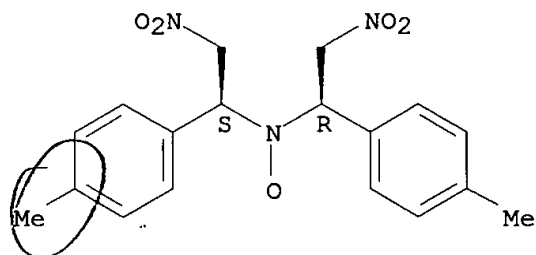
Relative stereochemistry.



RN 34940-04-0 CAPLUS

CN Nitroxide, bis[1-(4-methylphenyl)-2-nitroethyl], (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 34818-03-6 34818-04-7 34818-05-8

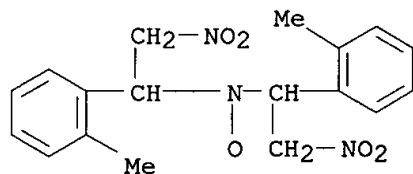
34818-06-9 34818-07-0

RL: PRP (Properties)

(ESR of)

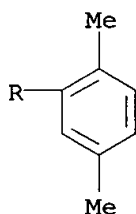
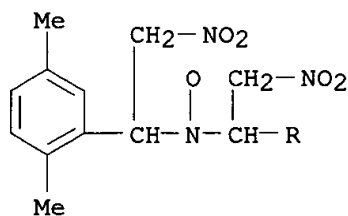
RN 34818-03-6 CAPLUS

CN Nitroxide, bis[1-(2-methylphenyl)-2-nitroethyl] (9CI) (CA INDEX NAME)



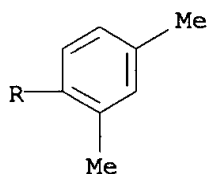
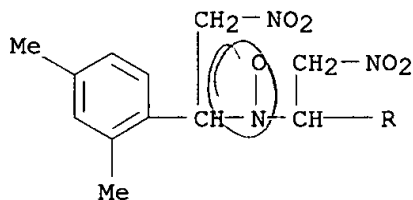
RN 34818-04-7 CAPLUS

CN Nitroxide, bis[1-(2,5-dimethylphenyl)-2-nitroethyl] (9CI) (CA INDEX NAME)



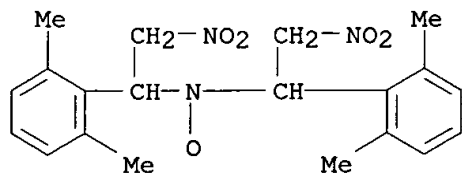
RN 34818-05-8 CAPLUS

CN Nitroxide, bis[1-(2,4-dimethylphenyl)-2-nitroethyl] (9CI) (CA INDEX NAME)



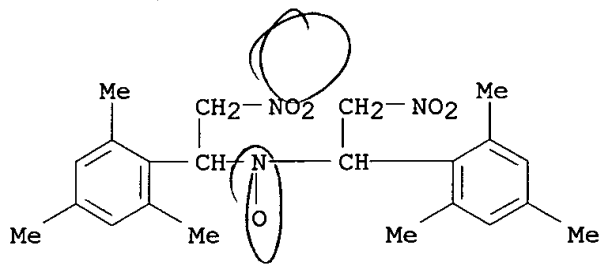
RN 34818-06-9 CAPLUS

CN Nitroxide, bis[1-(2,6-dimethylphenyl)-2-nitroethyl] (9CI) (CA INDEX NAME)



RN 34818-07-0 CAPLUS

CN Nitroxide, bis[2-nitro-1-(2,4,6-trimethylphenyl)ethyl] (9CI) (CA INDEX NAME)



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FILE 'REGISTRY' ENTERED AT 08:04:05 ON 04 JUN 2003

L1 STRUCTURE UPLOADED

L2 20 S L1 SSS SAM

L3 STRUCTURE UPLOADED

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L5 81 S L3 SSS FUL

FILE 'CAPLUS' ENTERED AT 08:06:32 ON 04 JUN 2003

L6 13 S L5

FILE 'CAOLD' ENTERED AT 08:07:05 ON 04 JUN 2003

=> s 15

L7 1 L5

=> d bib,hitstr



L7 ANSWER 1 OF 1 CAOLD COPYRIGHT 2003 ACS

AN CA55:1577c CAOLD

TI local anesthetics - (I) esters of 2-(dialkylamino)-1-phenylethanols, (II) esters of 2-amino-1-phenyl- and 2-amino-2-phenylethanols

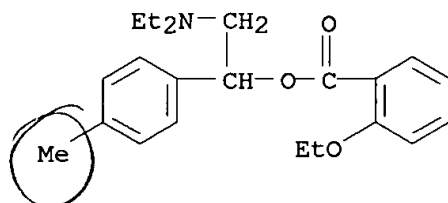
AU Shapiro, Seymour L.; Soloway, H.; Chodos, E.; Freedman, L.

IT 102700-75-4 110146-64-0 110245-22-2

110246-39-4

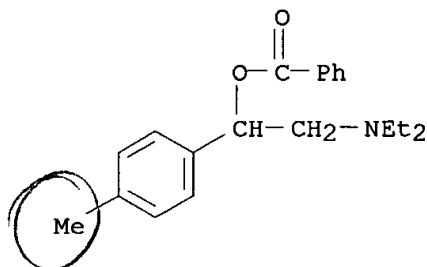
RN 102700-75-4 CAOLD

CN Benzoic acid, o-ethoxy-, .alpha.-(diethylaminomethyl)-p-methylbenzyl ester (6CI) (CA INDEX NAME)



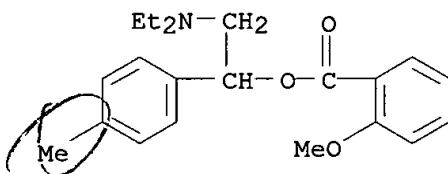
RN 110146-64-0 CAOLD

CN Benzyl alcohol, .alpha.-(diethylaminomethyl)-p-methyl-, benzoate (6CI) (CA INDEX NAME)



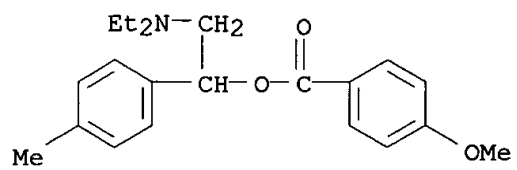
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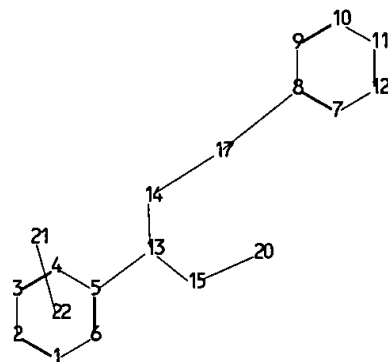
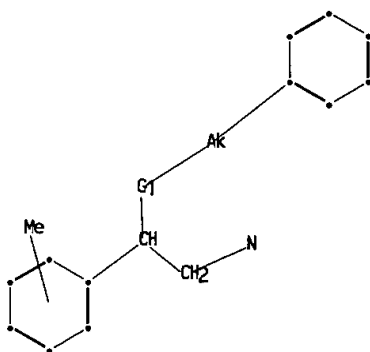
CN o-Anisic acid, .alpha.-(diethylaminomethyl)-p-methylbenzyl ester (6CI) (CA INDEX NAME)



RN 110246-39-4 CAOLD

CN p-Anisic acid, .alpha.-(diethylaminomethyl)-p-methylbenzyl ester (6CI) (CA INDEX NAME)





chain nodes :  
 13 14 15 17 20 21  
 ring nodes :  
 1 2 3 4 5 6 7 8 9 10 11 12  
 chain bonds :  
 5-13 8-17 13-14 13-15 14-17 15-20  
 ring bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12  
 exact/norm bonds :  
 8-17 13-14 14-17  
 exact bonds :  
 5-13 13-15 15-20  
 normalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12  
 isolated ring systems :  
 containing 1 : 7 :

G1:O,N

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
 12:Atom 13:CLASS 14:CLASS 15:CLASS 17:CLASS 20:CLASS 21:CLASS 22:CLASS  
 Element Count :  
 Node 17: Limited  
 C,C1-7